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PROBABILISTIC SHOCK INITIATION THRESHOLDS AND QMU APPLICATIONS

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Abstract

The Probabilistic Threshold Criterion (PTC) Project at LLNL develops phenomenological criteria for establishing margin of safety or performance margin on high explosive (HE) initiation in the high-speed impact regime, creating tools for safety assessment and design of initiation systems and HE trains in general. Until recently, there has been little foundation for probabilistic assessment of HE initiation scenarios. This work attempts to use probabilistic information that is available from both historic and ongoing tests to develop a basis for such assessment. Current PTC approaches start with the functional form of James' Initiation Criterion as a backbone, and generalize to include varying areas of initiation and provide a probabilistic response based on test data.

Recent work includes application of the PTC methodology to safety assessments involving a donor charge detonation and the need for assessment of a nearby acceptor charge's response, as well as flyer-acceptor configurations, with and without barriers. Results to date are in agreement with other less formal assessment protocols, and indicate a promising use for PTC-based assessments. In particular, there is interest in this approach because it supports the Quantified Margins and Uncertainties (QMU) framework for establishing confidence in the performance and/or safety of an HE system.

Introduction

The Ignition and Growth (I&G) Reactive Flow Model is a constitutive kinetics model that can be calibrated to match 50% threshold sensitivity of high explosives (HE).[1] Once tuned to a particular HE's response, I&G can be used to establish relative reactivity to a particular excitation, and can provide insight into how an HE responds to a stimulus. It is not a kinematic model in that no geometry of burn is imposed (as in program burn models), but truly dynamic in that each finite element "decides" how much to react based on its local state. As such, I&G is a rather expensive model to run, and when used in larger engineering finite element models, I&G can be computationally cost-prohibitive. In addition, I&G is tuned to an idealized 50% threshold and cannot directly provide the analyst with a sense of "margin from initiation" when needed.

In recent years, a simple approach has been proposed to get a sense of margin to initiation for high-speed impact problems. Hugh James of the Atomic Weapons Establishment, UK, proposed an initiation criterion that built upon the previous critical energy fluence criterion of Walker and Wasley.[2] In addition to sufficient work performed on a surface (energy fluence), James identified that sufficient specific kinetic energy was simultaneously required. James showed that there existed a hyperbolically-shaped criterion in energy fluence vs. specific kinetic energy space that separated initiation from non-initiation.[3] Hrousis (LLNL) proposed that one could define an initiation metric (J) based on James' Initiation Criterion, assume it to be randomly distributed due to sample variability and experimental uncertainty, and quantify a margin against initiation (or non-initiation) by knowing the distance from the 50% threshold criterion coupled with the uncertainty in the threshold based on experiments. This approach, though significantly more crude that full I&G, provides some simple engineering insight on the likelihood of SDT (shock-to-detonation transition) in an HE subjected to high speed impact. Combination of James' Criterion with an assumption about the initiation probabilistic distribution, and further amendments to account for diameter (2-D) effects results in a generalized "Probabilistic Threshold Criterion" (PTC) for future assessments.

Methods & Results

The James Initiation Criterion, as defined by James [3], is:

$$1 = \frac{E_c}{E} + \frac{\Sigma_c}{\Sigma}$$

where $\Sigma = \frac{1}{2}u^2$ and $E = pu\Delta t$.

In addition, $p =$ shock pressure, $u =$ particle velocity and $\Delta t =$ duration of shock. E, the energy fluence or work per unit area flowing into the HE, was originally defined by Walker & Wasley [2] for flat-topped shocks using a constant pressure, p, held over a finite time period, Δt. We suggest the following generalization:

$$\mathrm{E} = \int p\,u\;dt$$

This form is intended to be applicable to general time-varying pressure histories, as would be expected from shock input from a donor explosive or other initiator (such as an exploding bridgewire), as well as for flat topped shocks. The energy fluence, E, using the integral representation, and the specific kinetic energy, Σ, are easily calculated for material points in a hydrodynamic analysis code. Both E_c and Σ_c are critical values for those normalized energies, and are material properties intrinsic to the HE, functions of its formulation and local density.

Though phenomenological, the concept of James' Criterion makes intuitive sense. Sufficient energy fluence thorough a particular interface area is clearly needed for initiation, but it must occur before too much of it dissipates or transports away from the site of application. The local energy at the application site is captured by the Σ term, and if the needed energy fluence is not achieved before Σ dissipates, non-initiation is expected. It makes sense that there would exist a trade-off between magnitudes of E and Σ relative to their critical values, and thus the hyperbolic locus of points forming the initiation criterion. The cutoff concept introduced by Σ seems parallel to the run-distance required for detonation seen in POP-plots, and the relationship between James' Criterion and the POP-plot has been explored by James.[4]

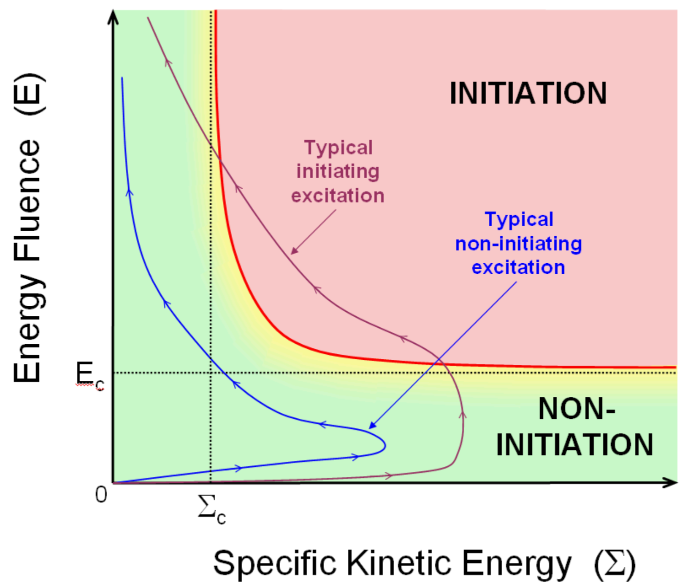

Figure 1. Concept of James' Initiation Criterion. Shock input is translated into E vs. Σ space for material points in the explosive. If the explosive experiences states above and to the right of the James' Criterion hyperbola, initiation is predicted.

Figure 1 illustrates the basic principle of James' Initiation Criterion: that when plotted in E vs. Σ space, initiating insults cause the HE to experience states above and to the right of the James Criterion hyperbola, while those that do not cause initiation remain below and to the left of the criterion. The principle suggests that marginal initiations correspond to traces that barely touch the criterion, while robust initiating systems (in performance mode) delve greatly into the initiation regime and very safe non-initiating scenarios stay far away from crossing the criterion. We suggest one way of quantifying HE excitation is to define a metric, J, whose level surfaces are everywhere parallel to the criterion, as follows:

$$\frac{1}{J} = \frac{E_c}{E} + \frac{\Sigma_c}{\Sigma}$$

We then identify $J_{\max}$, the largest numerical value of J experienced in the HE, and assert that $J_{\max}$ is a viable metric for predicting initiation, in the following way:

$J_{\max} = 1$ implies marginal initiation

$J_{\max} > 1$ implies initiation (performance), with margin

$J_{\max} < 1$ implies non-initiation (safety), with margin

For example, we consider the situation where an UF-TATB booster is lighting a larger charge of LX-17, shown in **Figure 2**. Both Fabry-Perot Velocimetry measurements and hydrocode predictions of the initiation system indicate differing pressure histories at different polar angles, as shown in **Figure 3**. To develop a bounding estimate of an uncertainty-normalized margin metric (or "QMU confidence factor," M/U), we see that at 85° polar angle, a $J_{\max}$ of 1.5 is obtained. Since our estimate of the uncertainty in the threshold J is about 0.1, our estimated $M/U = (1.5 - 1)/0.1 = 5$, which implies a very high level of confidence of initiation at 85°. This is not intended to be an exact calculation, but a preliminary engineering estimate of the robustness of the design.

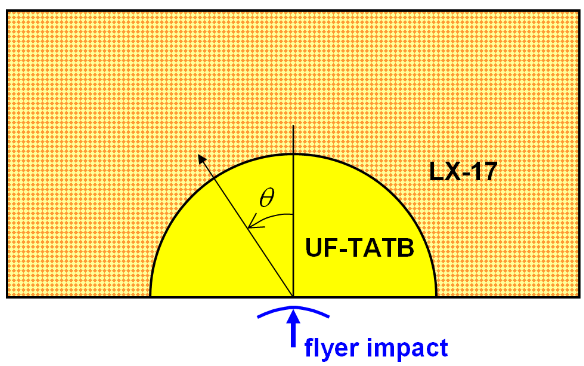

Figure 2. Simple IHE initiation system. A flyer impacts the UF-TATB booster and initiates it. The booster emits a shock into the surrounding LX-17 at different pressures and different times at varying polar angles, θ.

This method appears to work best for simple, one-dimensional scenarios, where a large, non-diverging, planar insult is approaching a large slab of HE. The method begins to break down as the excited diameter of HE decreases and approaches the order of the critical diameter. Decreasing excitation diameter causes the effective James Criterion to move up and to the right – it becomes harder to initiate. One way of capturing this effect is to quantify E_c and Σ_c as decreasing functions of excitation diameter (asymptotically approaching their 1-D values).

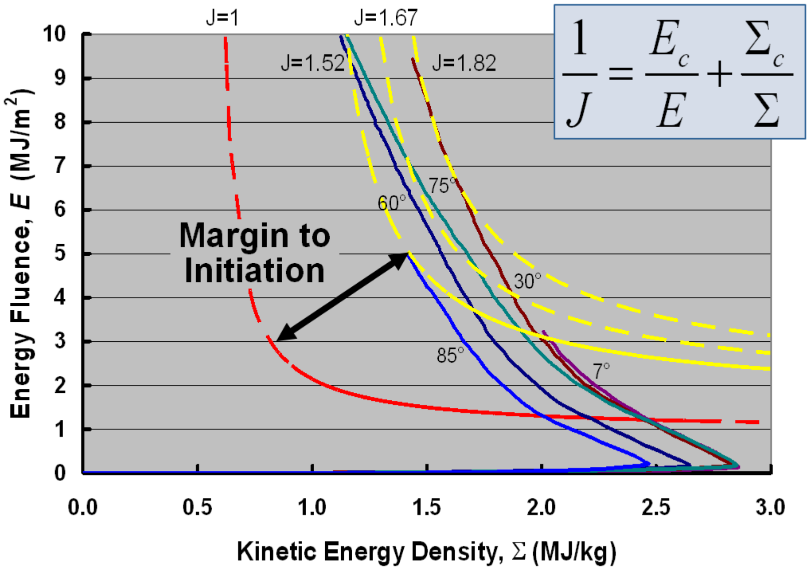

Figure 3. Example of a performance-mode application of a James' Criterion-based margin assessment. The curves marked with 7°, 30°, 60°, 75° and 85° are E-Σ histories of LX-17 excitation at those polar angles. The $J=1$ curve reproduces James' Criterion, as originally stated. The 85° E-S history is least robust of those shown, but can be shown to have ample margin in that it is tangent to the $J=1.52$ curve, and therefore the M/U for initiation is no less than 5. (This calculation is conservative in that the shock from the booster is diverging, though the 1-D James Criterion for LX-17 was not adjusted for that.)

For instance, consider the initiator for the above-mentioned UF-TATB booster, which is an explosively driven flyer, considerably larger than the critical diameter for UF-TATB, but not so large that the critical diameter effect can be ignored. For this scenario, we have tabulated experimental data both for 1-D initiation of UF-TATB, and at the diameter of its flyer initiator. In the 1-D case, $E_c = 0.20$ and $\Sigma_c = 0.51$. In the reduced flyer-diameter case, both values increase about 30%: $E_c = 0.26$ and $\Sigma_c = 0.67$. It is these increased values we use in estimating margins on the initiation of the UF-TATB in this system. The system is depicted in **Figure 4**, both in a performance mode, when the flyer is able to initiate the booster, and in a safety mode, where the flyer is blocked by a 1.5 mm steel barrier.

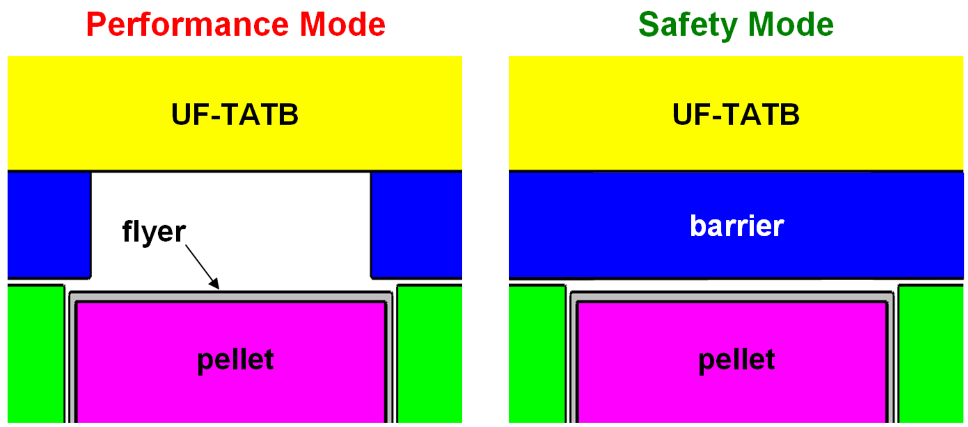

Figure 4. Simple pellet-driven flyer into UF-TATB booster initiation scheme. In performance mode, the pellet detonates, launching a flyer into the UF-TATB with great speed. In safety mode, a steel barrier blocks the flyer, and the shock attenuates greatly through the 1.5 mm of barrier thickness.

Historical tests were performed to quantify how much margin is present in the 1.5 mm barrier design. It was found that 0.1 mm of barrier thickness was sufficient to keep the UF-TATB from initiating, while 0.05 mm was not. These results were interpreted as a margin factor of $1.5/0.1 = 15$ "on thickness," since 15 times the needed thickness of barrier existed in the design. At present, we believe this to be an inappropriate way to quantify margin, as neither shock strength nor duration scale directly with the barrier thickness. Instead, we suggest the James Criterion-based approach suggested above, using the UF-TATB parameters at the diameter of the design. **Figure 5** shows the E and Σ history traces experienced by multiple material (Lagrangian) points in a hydrodynamic simulation of the 0.05 mm and 0.1 mm barrier tests. The quantity J is averaged over the area of the flyer, and it is found that the average $J_{\max}$ for the 0.05 mm case is 1.02 (suggesting initiation), and the average $J_{\max}$ for the 0.1 mm case is 0.97 (suggesting non-initiation). Both are near-marginal cases. Because the barrier thickness threshold experiments agree so well with the independent James Criterion-based margin approach, this provides some level of validation to the method.

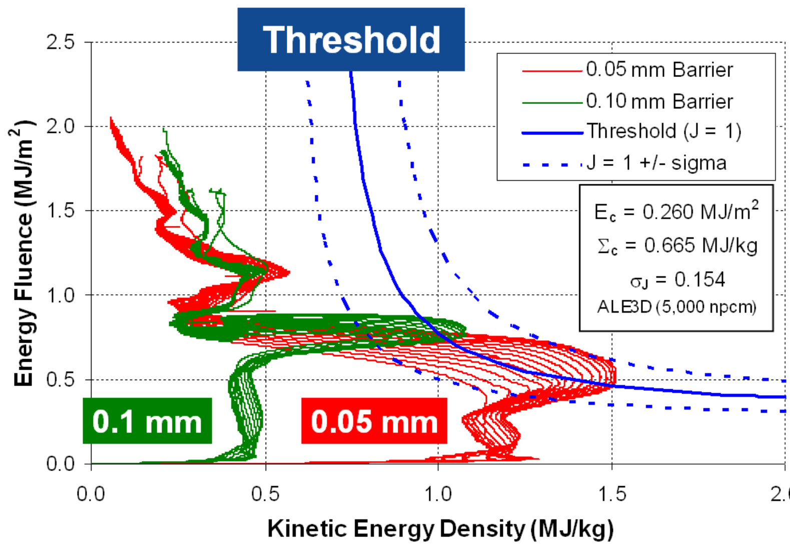

Figure 5. Comparison of near-threshold excitations with reduced-diameter UF-TATB James' Criterion threshold curve. E-Σ history traces for multiple material points over the excited diameter are plotted along with the threshold criterion. The average J_{max} for the 0.05 mm case is 1.02 and for the 0.1 mm case is 0.97, consistent with the experimental observation that these cases are just above and just below threshold.

It is also desirable to have an engineering sense of the probability of initiation based on J. The most important simplifying assumption to be made to accomplish this is the application of a probability distribution describing probability of initiation as a function of J. Analysis of experimental data for flyer-impact initiation of UF-TATB yields not only the E_c and Σ_c that place $J = 1$ at the 50% initiation point, but also σ_J, which is the best fitting one-sigma uncertainty in J, assuming it to be normally distributed. It is interesting to note that we calculate the best-fitting σ_J to be 0.15 for both the 1-D and reduced diameter cases. The σ_J parameter is most likely driven by experimental uncertainties, such as engineering tolerances, uncertainty and variability in flyer performance, etc. (epistemic uncertainty). Although it is also conceivable that it is affected by material-driven uncertainties as well, such as local variations in pressing density, variations in particle surface area, etc. (aleatory uncertainty). Both types of uncertainty are expected to exist in the designed application, as well as the experiment, and are assumed to be controlled to the same degree. This is hopefully a conservative assumption in both performance and safety modes, as the design application is likely to have a smaller (unknown) uncertainty than the threshold experiments. If so, the estimate of the σ_J in our calculations is large, bounding our M/U confidence factors and performance mode initiation probabilities (on the low side) and our safety mode initiation probabilities (on the high side).

Going back to our 1.5 mm barrier design example, **Figure 6** shows the calculated E - Σ history trace for the case where the full 1.5 mm barrier is in place, and the HE excitation caused by the small remaining shock that was not attenuated by the barrier. We see that the Lagrangian points in the UF-TATB experience excitations far below the James Criterion, and the maximum average J is 0.13. The safety M/U confidence factor is $(1-0.13)/0.15 = 5.8$, and using the normal distribution seen in the experimental threshold data, the predicted probability of initiation is less than 10^{-8}. **Figure 7** shows the calculated E - Σ history trace when no barrier is in place (performance mode). The maximum average J is 1.86, corresponding to a performance M/U confidence factor of 5.7 and a probability of non-initiation near 10^{-8}. These are intended to be engineering estimates only, confirming the robustness of the design in both performance and safety modes.

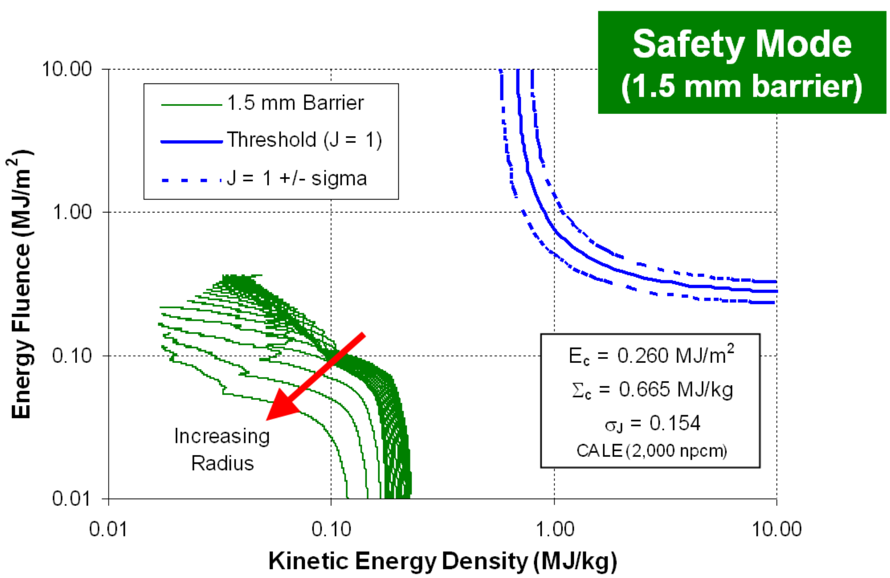

Figure 6. Comparison of 1.5 mm barrier excitation with reduced-diameter UF-TATB James' Criterion threshold curve. The average J_{max} for this case is 0.13 and the corresponding initiation probability is less than 10^{-8}.

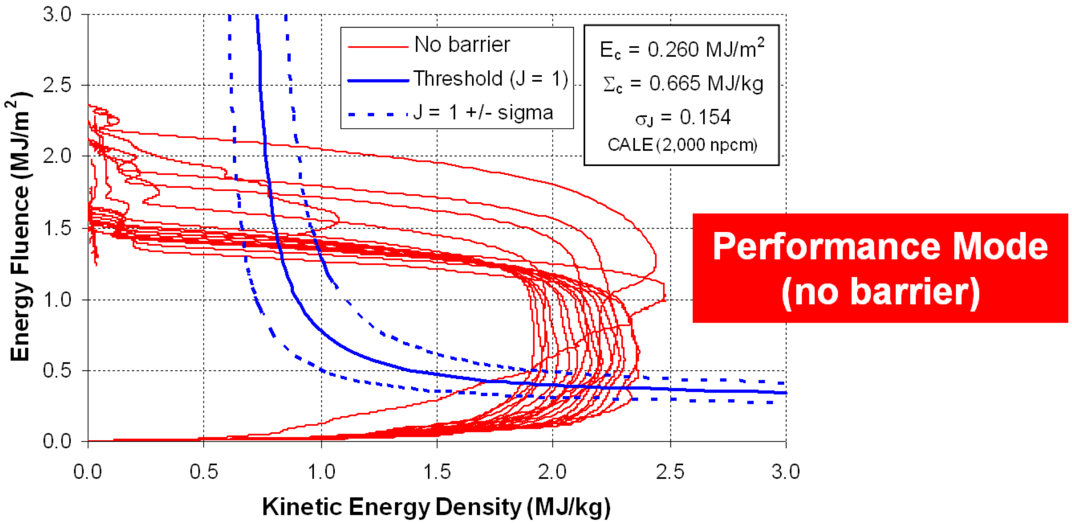

Figure 7. Comparison of "no barrier" performance mode excitation with reduced-diameter UF-TATB James' Criterion threshold curve. The average J_{max} for this case is 1.86 and the corresponding probability of non-initiation is near 10^{-8}.

Our current work focuses on further validation of the notion that non-flat pressure histories can be used with the James Criterion in the way described here. We are also working on refining the appropriate similar approach for initiation of LX-17. We are using Ignition & Growth Reactive Flow models (which tend to independently reproduce the James Criterion threshold curve) to extend to other excitation diameters. We have also been able to characterize E_c and Σ_c for LX-17 over a range of densities, and thus brought down our σ_J uncertainty to be even smaller than that of UF-TATB. One interesting note is that the corresponding probabilistic distribution curve does not appear to be symmetric (believed driven by initiation chemistry on the initiating side and experimental uncertainties on the non-initiating side). Other current work focuses on incorporating pressure history measurements via PDV (photonic Doppler velocimetry) into future initiation system performance measurements.

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